

REMARKS

This paper responds to the non-final Office Action dated April 20, 2006. In that Office Action, each of the pending claims was rejected under 35 U.S.C. § 112. Applicant has amended each of the pending independent claims to address the rejection, and submits that the claims are in condition for immediate allowance.

Comments on Information Disclosure Statement

The Office Action indicates that certain references in the Information Disclosure Statement of March 19, 2004 were not legible. Applicant has submitted herewith a Supplemental Information Disclosure Form attaching clean copies of each of the references.

Objections to Specification

The Office Action objects to three locations in the specification. Applicants have amended the specification as noted above, and believe that the amendments address two of the objections. The third objection relates to the use of the short-hand "MD" for molecular dynamics. The Office Action suggests that the term MD is not correlated with "molecular dynamics" in the specification, but Applicant notes that such a correlation is made at page 1, line 13. Applicant believes that such a correlation is sufficient to address the Office's concern, but is willing to make further clarifications if required by the Office.

Rejections Under 35 U.S.C. § 112

The Office Action rejects claims 37-72 under 35 U.S.C. § 112, para. 1. Applicant has amended the independent claims of this group (claims 37 and 55) to indicate that the ion is a monoatomic ion. Applicants note, however, that the simulation of the ion may be polyatomic. In particular, as noted in the pending application, such as at pages 7-10, a single atom ion may be more accurately simulated using a polyatomic representation (e.g., four atoms surrounding the actual atom) in the form of a virtual ion, rather than in a single atom form. In the polyatomic representation, the dummy atoms may mimic the vacant orbitals of the metal ion, and thereby

Applicant : Yuan-Ping Pang
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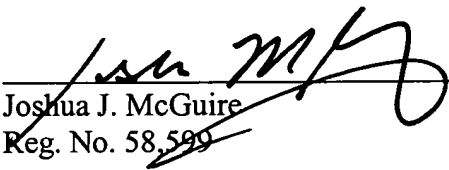
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produce a result that might otherwise not be obtained using other forms of molecular dynamics simulations. The recitation in the claim does not, of course, mean that the single atom ion may not be part of a larger structure. Therefore, Applicant believes that the present amendment adequately addresses the Office's rejection, and submits that the pending claims are in condition for allowance.

Enclosed is a \$510 check for the Petition for Extension of Time fee. Please apply any other charges or credits to deposit account 06-1050.

Respectfully submitted,

Date: 10/20/06



Joshua J. McGuire
Reg. No. 58,599

Fish & Richardson P.C.
60 South Sixth Street
Suite 3300
Minneapolis, MN 55402
Telephone: (612) 335-5070
Facsimile: (612) 288-9696